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TECHNICAL REPORT NO. 33

GENERATING FUNCTIONAL FOR ELECTRON-PHONON SYSTEMS FROM FUNCTIONAL

INTEGRALS WITH ONE-SIDED BOUNDARY CONDITIONS

by

Joao Florencio Jr.

University of Georgia
Department of Physics
Athens, Georgia 30602

November 5, 1986

Generating Functional for Electron-Phonon Systems from Functional

Integrals with One-Sided Boundary Conditions

João Florencio Jr.

Department of Physics and Astronomy, University of Georgia, Athens, GA 30602

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Matsubara perturbation formalism without using any results from the

standard operator method.

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The Matsubara formalism of perturbation theory at finite temperatures plays a distinctive role in the theory of many-body systems.[1] There one uses operator techniques to obtain thermal Green functions of the system as a perturbation expansion. Feynman rules can then be used to evaluate each term of the expansion. From the Green functions one obtain correlation functions, which are closely related to measurable quantities.

An alternative way to obtain the perturbation expansion is by the use of appropriate generating functionals for the thermal Green functions. Their forms are simple enough so that they can be postulated without further justification and yet they are known to reproduce the same results obtained by the operator method. There are, however, some attempts to derive generating functionals by using functional integral methods, namely in the work of Popov[2] and Casher et al[3]. These works, in turn, display some unsatisfactory features. In the work of Popov[2] the field operators are required form the beginning to be periodic (boson case) or antiperiodic (fermion case) in the inverse temperature. There requirements are by no means necessary to obtain the correct Green functions --which are indeed periodic (or antiperiodic) in the inverse temperature-- as one can easily verify this by using the standard operator method.[4] The derivation by Casher et al[3] makes use of an incorrect form of functional integrals in the holomorphic representation for bosons, in which the integrals used are over periodic paths.[5] Finally, it should be pointed out that none of these works give the explicit expression for the generating functional of the Matsubara Green functions which is the object of the present work.

In this paper we use the functional integral method described in Reference 6 to obtain the generating functional for the thermal Green functions of an electron-phonon system. The integration variables are c-numbers for the phonons and Grassmann numbers for the electrons, these variables satisfying one-sided boundary conditions at either 0 or β. The functional integrals used here are known to reproduce the correct partition functions of non-interacting systems of bosons and fermions. They were also used to obtain non-perturbative results for the molecular polaron with quadratic coupling model.[7]

Consider a system of electrons and phonons in a homogeneous medium of volume V. For simplicity we consider electrons with the same spin and phonons belonging to a single branch. The electron field operators $\hat{\psi}(x)$ and $\hat{\psi}^+(x)$ and the phonon field operator $\hat{\phi}(x)$ can be expressed by the following Fourier expansions[4]:

$$\hat{\psi}(x) = \frac{1}{\sqrt{V}} \sum_k e^{ikx} \hat{a}_k \ , \tag{1a}$$

$$\hat{\psi}^+(x) = \frac{1}{\sqrt{V}} \sum_k e^{-ikx} \hat{a}_k^+ \ , \tag{1b}$$

and

$$\hat{\phi}(x) = \frac{1}{\sqrt{V}} \sum_q \sqrt{\frac{\omega_q}{2}} \ (\hat{b}_q e^{iqx} + \hat{b}_q^+ e^{-iqx}) \ . \tag{1c}$$

The operators $\hat{a}_k$ and $\hat{a}_k^+$ are Fermi annihilation and creation operators, respectively, whereas $\hat{b}_q$ and $\hat{b}_q^+$ are the corresponding Bose operators. The quantities ω_q are the unperturbed phonon energies.

The Hamiltonian of the system is given by

$$\hat{H} = \hat{H}_0 + \hat{V} , \tag{2}$$

where

$$\hat{H}_0 = \sum_k \epsilon_k \hat{a}_k^+ \hat{a}_k + \sum_q \omega_q (\hat{b}_q^+ \hat{b}_q + \tfrac{1}{2}) \tag{3}$$

is the non-interacting part, and

$$\hat{V} = \int dx \; \hat{v}(\hat{\psi}^+(x), \hat{\psi}(x), \hat{\phi}(x)) \tag{4}$$

is the interaction between electrons and phonons. In the above, ϵ_k are the unperturbed single electron energies, and $\hat{v}$ is the interaction Hamiltonian density.

Now we introduce the temperature-dependent external sources ξ, ξ^* and η, which interact linearly with the electron and phonon operators as follows:

$$\hat{H}_I(\tau) = - \int dx \; (\hat{\psi}^+(x)\xi(x,\tau) + \xi^*(x,\tau)\hat{\psi}(x) + \hat{\phi}(x)\eta(x,\tau)) . \tag{5}$$

The sources ξ and ξ^* anticommute with the electron operators and among themselves, whereas η commutes with the phonon operators. These sources need not have actual physical meaning, and at the end we let them to vanish.

The grand-Hamiltonian $\hat{K}$ of the system in the presence of the sources is given by

$$\hat{K}(\tau) = \hat{H} + \hat{H}_I(\tau) - \mu\hat{N} , \tag{6}$$

where μ is the electron chemical potential, and $\hat{N} = \sum_k \hat{a}_k^+\hat{a}_k$ is the total number of electrons operator.

The generating functional is defined as the following functional of the external sources:

$$Z[\xi^*,\xi,\eta] = \text{Tr } \hat{\rho}[\xi^*,\xi,\eta] \ , \tag{7}$$

where

$$\hat{\rho}[\xi^*,\xi,\eta] = T_\tau \ \exp\{- \int_0^\beta \hat{K}(\tau)d\tau\} \tag{8}$$

is the density matrix in the presence of the sources. Here, T_τ is the temperature ordering operator. The trace operation can be performed in the holomorphic representation for the electrons and phonons, in which the electrons are represented by Grassmann numbers $--a_k$ and a_k^*-- and the phonons by c-numbers $--b_q$ and b_q^*. For details of holomorphic representations see, e.g., Faddeev and Slavnov[8] and references therein.

In the holomorphic representation, the right hand side of Eq.(7) is given by

$$\text{Tr } \hat{\rho}[\xi^*,\xi,\eta] = \iint \rho_{\xi^*,\xi,\eta}(b^*,a^*,b,a) \ \prod_q \exp(-b_q^*b_q) \ \frac{db_q^*db_q}{2\pi i}$$

$$\times \prod_k \exp(-a_k a_k^*) \ da_k da_k^* \ , \tag{9}$$

where $\rho_{\xi^*,\xi,\eta}(b^*,a^*,b,a)$ is the kernel of the density matrix operator, and the subscripts denote its functional dependence on the external sources. The density matrix kernel is represented by the following functional integral[6]:

$$\rho_{\xi^*,\xi,\eta}(b^*,a^*,b,a) = \int_{\substack{a_k^*(\beta)=a_k^* \\ a_k(0)=a_k}} \int_{\substack{b_q^*(\beta)=b_q^* \\ b_q(0)=b_q}} \exp\{\sum_q b_q^*(\beta)b_q(\beta) + \sum_k a_k^*(\beta)a_k(\beta)$$

$$+ \int_0^\beta \Big(- \sum_q b_q^*(u)\dot{b}_q(u) - \sum_k a_k^*(u)\dot{a}_k(u) - K(b^*(u),a^*(u),b(u),a(u),u)\Big) du\}$$

$$\times \Big(\prod_{q,u} \frac{db_q^*(u)db_q(u)}{2\pi i}\Big)\Big(\prod_{k,u} da_k^*(u)da_k(u)\Big) , \qquad (10)$$

where K is the <u>normal symbol</u>[8] of the operator $\hat{K}$, that is,

$$K = \sum_k (\epsilon_k-\mu)a_k^*a_k + \sum_q \omega_q(b_q^*b_q+\tfrac{1}{2}) + \int dx\, v(\Psi^*,\Psi,\Phi) - \int dx(\Psi^*\xi + \xi^*\Psi + \Phi\eta).$$

$$(11)$$

In the above expression, v is the normal symbol of the interaction density $\hat{v}$, and Ψ^*, Ψ and Φ are the normal symbols of the field operators $\hat{\Psi}^+$, $\hat{\Psi}$ and $\hat{\Phi}$, respectively. Notice that the functional integral is neither periodic nor antiperiodic in the inverse temperature, rather it obeys one-sided boundary conditions at either 0 or β.

The interaction part can be removed from the integrand, by using the following identity:

$$\exp\{ \int_0^\beta du\int dx \big(-v(\Psi^*,\Psi,\Phi) + \Psi^*(x,u)\xi(x,u) + \xi^*(x,u)\Psi(x,u) + \Phi(x,u)\eta(x,u)\big)\}$$

$$= \exp\{ - \int_0^\beta du\int dx\, v(\frac{\delta}{\delta\xi},\frac{\delta}{\delta\xi^*},\frac{\delta}{\delta\eta})\}\, \exp\{ \int_0^\beta du\int dx \big(\Psi^*(x,u)\xi(x,u)+\xi^*(x,u)\Psi(x,u)$$

$$+\Phi(x,u)\eta(x,u)\big)\} , \qquad (12)$$

where we have made the following replacements in v,

$$\psi^* \to \frac{\delta}{\delta\xi} \qquad \text{(right derivative)},$$

$$\psi \to \frac{\delta}{\delta\xi^*} \qquad \text{(left derivative)},$$

and

$$\phi \to \frac{\delta}{\delta\eta} \quad .$$

The exponential form containing v on the right hand side of Eq.(12) is to be understood as a power series expansion.

By using Eq.(12), the functional integrals for the electrons and phonons become decoupled from each other. The density matrix kernel assumes the following form:

$$\rho_{\xi^*,\xi,\eta}(b^*,a^*,b,a) = \exp\{-\int_0^\beta du \int dx \; v(\tfrac{\delta}{\delta\xi},\tfrac{\delta}{\delta\xi^*},\tfrac{\delta}{\delta\eta})\} \; \rho_\eta^{ph}(b^*,b) \; \rho_{\xi^*,\xi}^{el}(a^*,a) \; ,$$

$$(13)$$

where ρ_η^{ph} and $\rho_{\xi^*,\xi}^{el}$ are, respectively, the density matrix of non-interacting phonons and electrons in the presence of external sources. They are given, respectively, by

$$\rho_\eta^{ph}(b^*,b) = \int_{\substack{b_q^*(\beta)=b_q^* \\ b_q(0)=b_q}} \exp \; \Sigma_q \{b_q^*(\beta)b_q(\beta) + \int_0^\beta (-b_q^*(u)\dot{b}_q(u) - \omega_q(b_q^*(u)b_q(u)+\tfrac{1}{2})$$

$$- (b_q^*(u)\gamma_q(u) + b_q(u)\gamma_q^*(u)))du\} \; \prod_{q,u} \frac{db_q^*(u)db_q(u)}{2\pi i} \qquad (14)$$

and

$$\rho_{\xi^*,\xi}^{el}(a^*,a) = \int_{\substack{a_k^*(\beta)=a_k^* \\ a_k(0)=a_k}} \exp \sum_k \{a_k^*(\beta)a_k(\beta) + \int_0^\beta \left(-a_k^*(u)\dot{a}_k(u) - (\varepsilon_k-\mu)a_k^*(u)a_k(u)\right.$$

$$\left. - (a_k^*(u)\zeta_k(u) + \zeta_k^*(u)a_k(u))\right)du\} \prod_{k,u} da_k^*(u)da_k(u), \qquad (15)$$

where

$$\gamma_q(u) = - \frac{1}{\sqrt{V}}\sqrt{\frac{\omega_q}{2}} \int dx\ e^{-iqx}n(x,u)\ , \qquad (16a)$$

$$\gamma_q^*(u) = - \frac{1}{\sqrt{V}}\sqrt{\frac{\omega_q}{2}} \int dx\ e^{iqx}n(x,u)\ , \qquad (16b)$$

$$\zeta_k(u) = - \frac{1}{\sqrt{V}} \int dx\ e^{-ikx}\xi(x,u), \qquad (16c)$$

and

$$\zeta_k^*(u) = - \frac{1}{\sqrt{V}} \int dx\ e^{ikx}\xi^*(x,u)\ . \qquad (16d)$$

Both of the integrals (14) and (15) are Gaussian and can be evaluated exactly. Their solutions are simply the values of their integrands at the paths which extremize their actions, i.e., the arguments in the exponential forms[6]. The extremal conditions yield the equations

$$\dot{b}_q(u) + \omega_q b_q(u) + \gamma_q(u) = 0, \qquad b_q(0)=b_q \qquad (17a)$$

$$\dot{b}_q^*(u) - \omega_q b_q^*(u) - \gamma_q^*(u) = 0, \qquad b_q^*(\beta)=b_q^* \qquad (17b)$$

$$\dot{a}_k(u) + (\epsilon_k-\mu)a_k(u) + \zeta_k(u) = 0, \qquad a_k(0)=a_k \tag{17c}$$

and

$$\dot{a}_k^\star(u) - (\epsilon_k-\mu)a_k^\star(u) - \zeta_k^\star(u) = 0, \qquad a_k^\star(\beta)=a_k^\star. \tag{17d}$$

Their respective solutions are

$$b_q(u) = b_q e^{-\omega_q u} - \int_0^u e^{-\omega_q(u-s)}\gamma_q(s)ds, \tag{18a}$$

$$b_q^\star(u) = b_q^\star e^{\omega_q(u-\beta)} - \int_u^\beta e^{\omega_q(u-s)}\gamma_q^\star(s)ds, \tag{18b}$$

$$a_k(u) = a_k e^{-(\epsilon_k-\mu)u} - \int_0^u e^{-(\epsilon_k-\mu)(u-s)}\zeta_k(s)ds, \tag{18c}$$

and

$$a_k^\star(u) = a_k^\star e^{(\epsilon_k-\mu)(u-\beta)} - \int_u^\beta e^{(\epsilon_k-\mu)(u-s)}\zeta_k^\star(s)ds. \tag{18d}$$

Notice that neither these extremal paths nor their respective equations are complex conjugate pairs.

The values of the integrals (14) and (15) are then given, respectively, by

$$\rho_n^{ph}(b\star,b) = \exp\{-\sum_q \frac{\beta\omega_q}{2}\}\exp\sum_q\{b_q^\star b_q e^{-\beta\omega_q} - b_q^\star e^{-\beta\omega_q}\int_0^\beta e^{\omega_q u}\gamma_q(u)du$$

$$- b_q\int_0^\beta e^{-\omega_q u}\gamma_q^\star(u)du + \int_0^\beta du\int_0^u ds\, e^{-\omega_q(u-s)}\gamma_q^\star(u)\gamma_q(s)\} \tag{19}$$

and

$$\rho^{el}_{\xi^*,\xi}(a^*,a) = \exp\Sigma_k \{a^*_k a_k e^{-\beta(\epsilon_k-\mu)} - a^*_k e^{-\beta(\epsilon_k-\mu)} \int_0^\beta e^{(\epsilon_k-\mu)u}\zeta_k(u)du$$

$$- (\int_0^\beta e^{-(\epsilon_k-\mu)u}\zeta^*_k(u)du)a_k + \int_0^\beta du \int_0^u ds\ e^{-(\epsilon_k-\mu)(u-s)}\zeta^*_k(u)\zeta_k(s)\} \ .$$

$$(20)$$

These are the final results for the density matrix kernels of
non-interacting phonons and electrons in the presence of external
sources. Next we use the trace formulae to obtain the following
partition functions:

$$Z^0_{ph}[\eta] = \int \rho^{ph}_\eta(b^*,b)\exp\{-\Sigma_q b^*_q b_q\}\ \Pi_q \frac{db^*_q db_q}{2\pi i}$$

$$= (\ \Pi_q \frac{e^{-\frac{1}{2}\beta\omega_q}}{1-e^{-\beta\omega_q}}\ )\exp\{\Sigma_q ((N^B_q+1)\int_0^\beta du\int_0^u ds\ e^{-\omega_q(u-s)}\gamma^*_q(u)\gamma_q(s)$$

$$+ N^B_q \int_0^\beta du\int_u^\beta ds\ e^{-\omega_q(u-s)}\gamma^*_q(u)\gamma_q(s))\} \qquad (21)$$

and

$$Z^0_{el}[\xi^*,\xi] = \int \rho^{el}_{\xi^*,\xi}(a^*,a)\exp\{-\Sigma_k a_k a^*_k\}\ \Pi_k da_k da^*_k$$

$$= (\ \Pi_k(1+e^{-\beta(\epsilon_k-\mu)})\ )\exp\{\Sigma_k (\int_0^\beta du\int_0^u ds\ e^{-(\epsilon_k-\mu)(u-s)}\zeta^*_k(u)\zeta_k(s)$$

$$- N^F_k \int_0^\beta du\int_0^\beta ds\ e^{-(\epsilon_k-\mu)(u-s)}\zeta^*_k(u)\zeta_k(s))\} \ , \qquad (22)$$

where

$$N^B_q = \frac{1}{e^{\beta\omega_q} - 1}$$

$$N_k^F = \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1}$$

are, respectively, the familiar Bose and Fermi distribution functions. Notice that the dependence of the partition functions on η, ξ^* and ξ is implicitly understood in the above expressions due to Eqs.(16a-d).

We now use the following identities

$$\sum_q (N_q^B + 1) \int_0^\beta du \int_0^u ds \; e^{-\omega_q(u-s)} \gamma_q^*(u) \gamma_q(s) = \frac{1}{2} \sum_q (N_q^B + 1) \int_0^\beta du \int_0^\beta ds \; e^{-\omega_q |u-s|} \gamma_q^*(u) \gamma_q(s),$$

$$(23a)$$

$$\sum_q N_q^B \int_0^\beta du \int_u^\beta ds \; e^{-\omega_q(u-s)} \gamma_q^*(u) \gamma_q(s) = \frac{1}{2} \sum_q N_q^B \int_0^\beta du \int_0^\beta ds \; e^{\omega_q |u-s|} \gamma_q^*(u) \gamma_q(s)$$

$$(23b)$$

and

$$\sum_k \int_0^\beta du \int_0^u ds \; e^{-(\epsilon_k - \mu)(u-s)} \zeta_k^*(u) \zeta_k(s) = \sum_k \int_0^\beta du \int_0^\beta ds \; e^{-(\epsilon_k - \mu)(u-s)} \zeta_k^*(u) \zeta_k(s) \theta(u-s)$$

$$(23c)$$

where θ is the step function, together with Eqs.(16a-d) to express the partition functions (21) and (22) in the following forms:

$$Z_{ph}^0[\eta] = \left(\prod_q \frac{e^{-\frac{1}{2}\beta\omega_q}}{1 - e^{-\beta\omega_q}} \right) \exp\{ \frac{1}{2} \int_0^\beta du \int_0^\beta ds \int dx \int dy \; \eta(x,u) \frac{1}{V} \sum_q \frac{\omega_q}{2} ((N_q^B + 1) e^{iq(x-y)} e^{-\omega_q |u-s|}$$

$$+ N_q^B e^{iq(x-y)} e^{\omega_q |u-s|}) \eta(y,s) \}$$

$$(24)$$

and

$$Z_{el}^0[\xi^*,\xi] = \left(\prod_k (1 + e^{-\beta(\epsilon_k - \mu)}) \right) \exp\{ \int_0^\beta du \int_0^\beta ds \int dx \int dy$$

$$\times \xi^*(x,u) \frac{1}{V} \sum_k e^{ik(x-y)} e^{-(\epsilon_k - \mu)(u-s)} (\theta(u-s) - N_k^F) \xi(y,s) \} \quad .$$

$$(25)$$

Notice that the unperturbed thermal Greem functions for electrons and phonons appear explicitly in the above expressions. In addition , the pre-exponential forms are simply the unperturbed partition functions. More explicitly,

$$Z_{ph}^0[\eta] = Z_{ph}^0 \exp\{-\tfrac{1}{2} \int_0^\beta du \int_0^\beta ds \int dx \int dy \ \eta(x,u)D^{(0)}(x,u;y,s)\eta(y,s)\} \quad (26)$$

and

$$Z_{el}^0[\xi^*,\xi] = Z_{el}^0 \exp\{- \int_0^\beta du \int_0^\beta ds \int dx \int dy \ \xi^*(x,u)G^{(0)}(x,u;y,s)\xi(y,s)\} \ ,$$

$$(27)$$

where

$$Z_{ph}^0 = \prod_q \frac{e^{-\tfrac{1}{2}\beta\omega_q}}{1-e^{-\beta\omega_q}} \ , \quad (28)$$

$$Z_{el}^0 = \prod_k (1 + e^{-\beta(\epsilon_k-\mu)}) \ , \quad (29)$$

$$D^{(0)}(x,u;y,s) = -\frac{1}{2V}\sum_q \omega_q ((N_q^B+1)e^{iq(x-y)}e^{-\omega_q|u-s|} + N_q^B e^{iq(x-y)}e^{\omega_q|u-s|}) \ ,$$

$$(30)$$

and

$$G^{(0)}(x,u;y,s) = -\frac{1}{V}\sum_k e^{ik(x-y)}e^{-(\epsilon_k-\mu)(u-s)}(\Theta(u-s) - N_k^F). \quad (31)$$

The above expressions for the unperturbed phonon Green function $D^{(0)}$ and the electron Green function $G^{(0)}$ are the same found in textbooks.[9] Hotice that they were obtained here strictly from functional integral methods. There was no assumption made concerning periodicity or antiperiodicity of the field operators in the imaginary time, yet these

Green functions do obey periodicity $--D^{(0)}--$ and antiperiodicity $--G^{(0)}--$ conditions.

Finally, by combining the above results we arrive at the final expression for the generating functional for the interacting system:

$$Z[\xi^{*},\xi,\eta] = Z^{0} \exp\{- \int_{0}^{\beta} du \int dx \ v(\frac{\delta}{\delta\xi},\frac{\delta}{\delta\xi^{*}},\frac{\delta}{\delta\eta})\}$$

$$x \exp\{- \frac{1}{2} \int_{0}^{\beta} du \int_{0}^{\beta} ds \int dx \int dy \ \eta(x,u)D^{(0)}(x,u;y,s)\eta(y,s)$$

$$- \int_{0}^{\beta} du \int_{0}^{\beta} ds \int dx \int dy \ \xi^{*}(x,u)G^{(0)}(x,u;y,s)\xi(y,s)\} \ , \qquad (32)$$

where $Z^{0} = Z_{ph}^{0}Z_{el}^{0}$.

The partition function is obtained by first expanding the form containing the interaction v in a power series, and then performing the functional derivatives required in each term of the series and, finally, setting the sources equal to zero. Of course, one still is left with integrals over the spatial coordinates and the inverse temperature. This procedure amounts to summing all possible diagrams with no external lines.

The two-point Green functions for the electrons and phonons are obtained, respectively, by

$$G(x_{1},\tau_{1};x_{2},\tau_{2}) = - \frac{1}{Z} \frac{\delta^{2}Z}{\delta\xi^{*}(x_{1},\tau_{1})\delta\xi(x_{2},\tau_{2})}\bigg|_{\xi^{*}=\xi=\eta=0} \qquad (33)$$

and

$$D(x_{1},\tau_{1};x_{2},\tau_{2}) = - \frac{1}{Z} \frac{\delta^{2}Z}{\delta\eta(x_{1},\tau_{1})\delta\eta(x_{2},\tau_{2})}\bigg|_{\xi^{*}=\xi=\eta=0} \ . \qquad (34)$$

The diagram expansions of these Green functions will contain only connected diagrams with two external lines. As usual, each line in a given diagram is associated with an unperturbed Green function and the vertices are associated with the interaction v. The coordinates x_1 and x_2 denote the free ends of the external lines at τ_1 and τ_2, respectively. In these expansions, Wick's theorem is automatically satisfied. Finally, it should be pointed out that Green functions with many-points can also be obtained from (32).

To summarize, we have derived the explicit expression of the generating functional for the temperature dependent perturbation theory of an electron-phonon system. The form (32) which insofar has only been used heuristically is now indeed justified. One should also notice that no use of prior results from the operator method was required to the derivation of the generating functional. In a forthcoming article we use techniques of functional integrals in the holomorphic representation to show how to obtain non-perturbative expansions for the partition functions of systems of bosons and fermions.

ACKNOWLEDGMENTS

REFERENCES

1. T. Matsubara, Prof. Theor. Phys. $\underline{14}$, 351 (1953).

2. A. Casher, D. Lurié, and M. Revzen, J. Math. Phys. $\underline{9}$, 1312 (1968).

3. V. N. Popov, Functional Integrals in Quantum Field Theory and Statistical Physics (Dordrecht: Reidel, 1983).

4. See, e.g., A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinsky, Methods of Quantum Field Theory in Statistical Physics (Englewood Cliffs: Prentice-Hall, 1963).

5. In the passage from Eq.(7) to Eq.(8) of Ref. 2, the authors mislabel some of the quantities involved: There is no justification for setting $\alpha_0 = \alpha_N$ in some terms while leaving the combination $\bar{\alpha}_0 \alpha_1$ unchanged.

6. J. Florencio and B. Goodman, Phys. Rev. B $\underline{34}$, 3634 (1986).

7. J. Florencio and B. Goodman, Phys. Rev. B $\underline{34}$, 3639 (1986).

8. L. D. Faddeev and A. A. Slavnov, Gauge Fields (Reading: Benjamin/ Cummings, 1980).

9. The form (30) can be found, for instance, in Ref. 1, p. 103, whereas the form (31) is in G. Mahan, Many-Particle Physics (Plenum: New York, 1981), p. 130.

A. XY and TI models in higher dimensions at infinite temperature.

The time evolution in the XY model is expected to be quite different
from that in the TI model since the two models are inequivalent. If, however,
the strength of the external field B in the one-dimensional TI model is
made to approach the coupling constant J, the time evolution becomes
identical to that in the one-dimensional XY model. We have shown that
when B = J, the geometric structure of the Hilbert spaces of S_j^x in the
TI and XY models become identical. The two structures are not identical
at any other values of B. It has been established that the form of the
time evolution is a unique function of the geometric structure of the
realized Hilbert space.[7] Hence one can understand the origin of the
coincidence in the time evolution of S_j^x at this particular value of B.
In addition, the realized recurrence relation turns out to be simple
enough to permit an analytic solution for the entire family of the
relaxation functions.

For the XY and TI models in higher dimensions, e.g. d = 2, one does
not presently know anything about their time evolution. While the
analytic solution for it poses a challenge to any method, there is a simpler,
perhaps more immediate problem. That is, whether the coincidence in the
time evolution is unique to one dimension, or whether it also exists in
higher dimensions possibly with some d-dependent values for B. This problem
can be readily tackled by the method of recurrence relations, since the
recurrants can be calculated in higher dinensions. According to the method
of recurrence relations, it is then sufficient to compare the geometric
structures of the realized Hilbert spaces and to find, it exists, the
value of B for which the two structures become identical to each other.[14,15]

END

1—81

DTIC